



Polymers under Multiple Constraints

Polymer- & Soft-Matter-Seminar

Tuesday,
26st January
2016

at: 5.15pm

VDP4 1.27,
Von-
Danckelmann-
Platz 4,
06120 Halle

Prof. Lillian Chong

(University of Pittsburgh, Department of Chemistry)

“Enhanced Sampling of Pathways and Kinetics of Rare Events using Weighted Ensembles of Trajectories”

The weighted ensemble (WE) path sampling strategy orchestrates quasi-independent parallel simulations that are run with intermittent communication to enhance sampling of rare events such as protein conformational changes, folding, and binding. Trajectories are pruned or replicated in a way that encourages sampling of under-explored regions without biasing the dynamics. I will present recent advances in both WE methodology and software along with applications to protein folding and binding processes in the generation of pathways, free energy landscapes, and rate constants.

